

Matrix-Product based Projected Wave Functions Ansatz for Quantum Many-Body Ground States

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We develop a new projected wave function approach which is based on projection operators in the form of matrix-product operators (MPOs). Our approach allows to variationally improve the short range entanglement of a given trial wave function by optimizing the matrix elements of the MPOs while the long range entanglement is contained in the initial guess of the wave function. The optimization is performed using standard variational Monte Carlo techniques. We demonstrate the efficiency of our approach by considering a one-dimension model of interacting spinless fermions. In addition, we indicate how to generalize this approach to higher dimensions using projection operators which are based on tensor products.

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One of the basic problems in physics is to find the ground state of strongly correlated electron systems. These are of central importance in several areas of science and technology, including solid state physics, quantum chemistry as well as nanotechnology. Analytical exact solutions are only available in few cases and one thus often relies on numerical studies. Efficient numerical methods also exist only for special cases. Quantum Monte Carlo (QMC) simulations [1] are for instance only efficient in the absence of any negative sign problem which occurs in most fermionic and frustrated systems. By contrast, exact diagonalizations are applicable in general fermionic models. However, the size of the corresponding Hilbert space grows exponentially with the system size and consequently only very small systems can be considered. In one dimensional systems, very accurate results have been obtained using the density matrix renormalization group (DMRG) [2]. The DMRG algorithm is closely related to the concept of matrix-product states (MPS) [3, 4] which can be generalized to higher dimensions using tensor-product states (TPS) [5]. Different TPS based or related approaches have been introduced recently, e.g., the projected entangled pair states (PEPS) [6, 7], string-bond states [8], scale-renormalized MPS [9], tensor entanglement renormalization group (TRG) [10, 11], correlator-product states [12, 13] and entangled-plaquette states [14–16]. It has been shown that Monte Carlo sampling in combination with MPS or TPS yields an efficient method to simulate spin systems [17, 18]. Although there exist applications to fermionic systems as well, the large amount of entanglement in fermionic wave functions is very difficult to capture, see e.g., Refs. [19, 20].

In this Letter, we propose a novel construction of trial wave functions to efficiently represent ground states of correlated spin and electronic systems. Our starting point is a known wave function which we use as a first approximation of the ground state, e.g., a mean-field wave function or any other better guess we might have. We then introduce projection operators represented in terms

of matrix-product operators (MPOs) [21–23] which are the operator analogue of MPS. The quality of the trial wave function can then be successively improved by increasing the dimension of the matrices used in the MPO. We will refer to these states as *matrix-product projected states (MPPS)*. Expectation values of physical observables are computed using Monte Carlo sampling. We use a variational Monte Carlo (VMC) scheme to optimize the MPO by minimizing the energy. The proposed MPPS approach can be generalized to higher dimensions by using tensor-product based projection-operators. Furthermore, the fermionic structure of the wave function can be incorporated by using, e.g., a simple Slater determinant constructed from mean-field Hamiltonians. This approach can work for frustrated or fermionic systems which cannot be dealt with using QMC. We discuss the approach for simplicity for the case of a one-dimensional system in detail and then indicate how to generalize it to higher dimensions.

The MPS representation of a quantum state on a chain of length L with periodic boundary condition is given by

$$|\psi^{\text{MPS}}\rangle = \sum_{j_1, \dots, j_L=1}^d \text{Tr} \left(\hat{A}_{[1]}^{j_1} \hat{A}_{[2]}^{j_2} \dots \hat{A}_{[L]}^{j_L} \right) |j_1\rangle \dots |j_L\rangle \quad (1)$$

where $\hat{A}_{[k]}^{j_k}$ are $\chi \times \chi$ matrices. The physical index $j_k = 1 \dots d$ represents d local states at site k . This state can be formally rewritten as

$$|\psi^{\text{MPS}}\rangle = \sum_{j_1, \dots, j_L=1}^d \text{Tr} \left(P_{[1]}^{j_1} P_{[2]}^{j_2} \dots P_{[L]}^{j_L} \right) |\phi_0^{\text{Product}}\rangle \quad (2)$$

in terms of the projector MPOs, $P_{[k]}^{j_k} (\equiv \hat{A}_{[k]}^{j_k} |j_k\rangle \langle j_k|)$, and $|\phi_0^{\text{Product}}\rangle$ is a site-factorized (product) state defined as

$$|\phi_0^{\text{Product}}\rangle \equiv \prod_{k=1}^L \left(\sum_{j_k=1}^d |j_k\rangle \right) = \sum_{j_1, \dots, j_L=1}^d |j_1\rangle \dots |j_L\rangle. \quad (3)$$

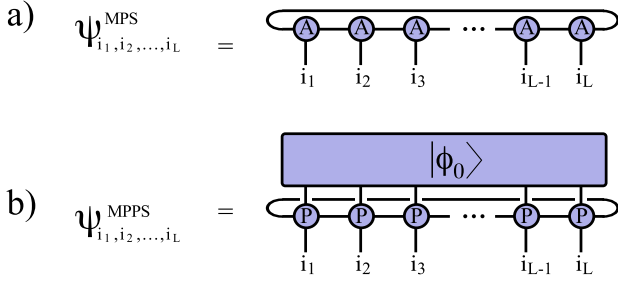


FIG. 1: (Color online) Schematic representation of a) a matrix-product state (MPS) and b) a matrix-product projected state (MPPS) with periodic boundary condition in a one-dimensional system. $|\phi_0\rangle$ is a guess to approximate for the trial wave function $|\psi\rangle$.

Clearly, any site-factorized state can be represented using $\chi = 1$ matrices which simply renormalize the weight for local states on each site individually. The entire entanglement in $|\psi^{\text{MPS}}\rangle$ is expressed by the matrices $\hat{A}_{[k]}^{j_k}$ and thus a more entangled state requires a larger χ . The bond dimension χ needed scales exponentially with the entanglement entropy S , with $S(= -\text{Tr} \rho_{\text{red}} \log \rho_{\text{red}})$ being the von-Neumann entropy of the reduced density matrix ρ_{red} . The success of the MPS representation in one dimensional systems is based on the fact that the entanglement in ground-state wave functions is low and thus they can usually be well approximated using a small bond dimension χ [5]. The main idea of this letter is to choose an initial wave function $|\phi_0\rangle$ which is already a better approximation of the ground state than the site-factorized state $|\phi_0^{\text{Product}}\rangle$ in Eq. (2). The improvement over an MPS representation is that a part of the entanglement is contained in $|\phi_0\rangle$. In other words, the projector MPOs only require modifying the local entanglement since the long range entanglement is already included in $|\phi_0\rangle$. This yields a much faster convergence in terms of the bond dimension compared to MPS (see the example discussed below). Furthermore, it allows us to express a larger class of states than MPS. In particular states which violate the area law, e.g., critical states, can be represented by using the MPPS approach. A pictorial representation which compares the MPS with the MPPS is given in Fig. 1.

As a specific example, we now discuss a model of spinless fermions at half-filling and show that the trial wave function is substantially improved over the standard MPS approach by choosing $|\phi_0\rangle$ to be a mean-field Slater determinant. The Hamiltonian is given by

$$H = -t \sum_i \left(c_i^\dagger c_{i+1} + H.c. \right) + V \sum_i \hat{n}_i \hat{n}_{i+1}, \quad (4)$$

where $\hat{n}_i = c_i^\dagger c_i$ and $V, t > 0$. Using the Jordan-Wigner transformation, the model is equivalent to the XXZ spin-1/2 Hamiltonian on the chain $H = \sum_{\langle ij \rangle} \left[\frac{J_\perp}{2} (s_i^+ s_{i+1}^- + s_i^- s_{i+1}^+) + \frac{J_z}{4} (s_i^z + 1) \cdot (s_{i+1}^z + 1) \right]$

where $s_i^\pm = \frac{s_i^x \pm i s_i^y}{2}$, $s_i^{x,y,z}$ are the Pauli matrices and are related to the fermions by $s_i^z = 2n_i - 1$, $s_i^+ = c_i^\dagger$, and $s_i^- = c_i$. Thus $J_z = V$ and $J_\perp = -2t$. The discussion below will be largely in terms of the fermionic model, although all the results are valid for the spin system as well.

In the non-interacting case (i.e., $V = 0$), the Hamiltonian (4) has a simple ground-state wave function which we choose as the initial wave function for the MPPS:

$$|\phi_0^{\text{Slater}}\rangle = \prod_{\vec{k}}^{\epsilon_{\vec{k}} < \epsilon_F} c_{\vec{k}}^\dagger |0\rangle = \sum_{j_1, \dots, j_L} S_{j_1, \dots, j_L} |j_1\rangle \dots |j_L\rangle. \quad (5)$$

Here ϵ_F denotes the Fermi energy, $\epsilon_{\vec{k}}$ is the dispersion relation and the local states are given by $j_k = 0, 1$. S_{j_1, \dots, j_L} is the Slater determinant for the configuration $|j_1\rangle \dots |j_L\rangle$. Using this initial wave function, the MPPS Ansatz reads

$$\begin{aligned} |\psi^{\text{MPPS}}\rangle &= \sum_{j_1, \dots, j_L} \text{Tr} \left(P_{[1]}^{j_1} \dots P_{[L]}^{j_L} \right) |\phi_0^{\text{Slater}}\rangle \\ &= \sum_{j_1, \dots, j_L} \text{Tr} \left(\hat{A}_{[1]}^{j_1} \dots \hat{A}_{[L]}^{j_L} \right) S_{j_1, \dots, j_L} |j_1\rangle \dots |j_L\rangle. \end{aligned} \quad (6)$$

There are two points in parameter space at which the ground-state wave function can be represented exactly with $\chi = 1$. Firstly, if $V = 0$, the ground state is given by $|\phi_0^{\text{Slater}}\rangle$ and thus does not require any modifications (i.e., $\hat{A}_{[k]}^{j_k} = 1$ for all k and j_k). Secondly, if $V \rightarrow \infty$, the ground state is a two-fold degenerate charge density wave (CDW) state (which is a product state in this limit). This state is simply obtained by choosing for example $\hat{A}_{[2k]}^1 = \hat{A}_{[2k+1]}^0 = 1$ for all k (all other elements being zero) – everything except one of the two CDW states is projected out from the Slater determinant. Note that in the former case, the state has algebraic correlations and thus an MPS requires a bond dimension which roughly scales linearly with the system size [24]. In the latter case, the MPS can also represent the ground state with $\chi = 1$.

Additionally, we consider for comparison another popular variational state with density-density Jastrow correlation factor. The Jastrow-type wave function can be defined as

$$|\psi^{\text{Jastrow}}\rangle = \exp \left(\sum_{i < j} \eta_{ij} \hat{n}_i^h \hat{n}_j^h \right) |\phi_0^{\text{Slater}}\rangle \quad (7)$$

with $\eta_{ij} \equiv \ln \left(r_{ij}^\alpha v_\beta^{\delta_{j,i+\beta}} \right)$. Here $r_{ij} = \left| \sin \left(\frac{\pi}{L} (x_i - x_j) \right) \right|$ and $\hat{n}_i^h = 1 - \hat{n}_i$. The two parameters v_β with the nearest and second-nearest neighbor indices β are for short range hole-hole repulsion if these values are less than 1. The factor r_{ij}^α is for long range correlations and repulsive if α is positive. In fact, we could use the optimized $|\psi^{\text{Jastrow}}\rangle$

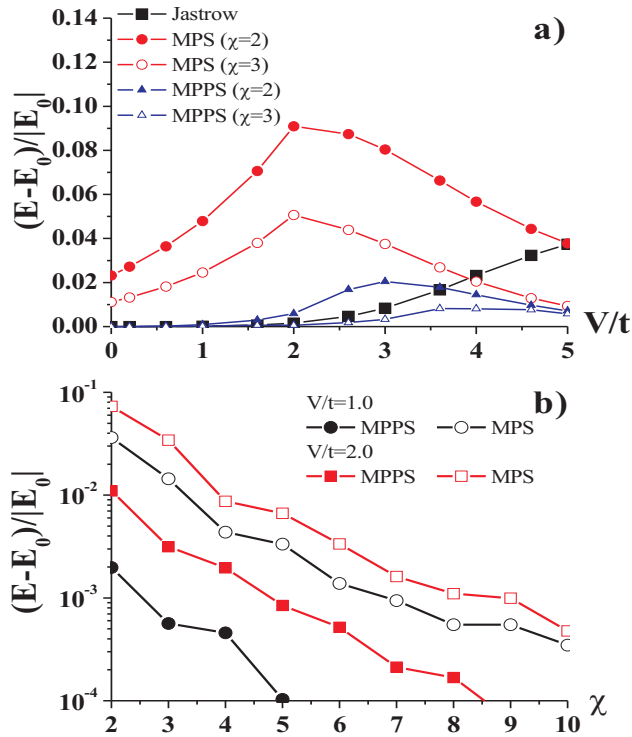


FIG. 2: (Color online) a) Comparison of the optimized energies for different trial states with exact diagonalization results for the $t-V$ model on a $L = 18$ chain with periodic boundary condition. b) Comparison of the optimized energies with infinite time-evolving block decimation results for different bond dimensions χ using the MPS and the MPPS for $V/t = 1, 2$ on a $L = 202$ chain. E_0 is the exact ground-state energy.

as the initial wave function for the MPPS approach (instead of $|\phi_0^{\text{Slater}}\rangle$). However, here we use $|\psi^{\text{Jastrow}}\rangle$ only as a benchmark to compare to the Slater determinant based MPPS.

We now use the VMC method to optimize the energy using the three different trial wave functions (MPS, MPPS and Jastrow) and to compute their correlation functions as well. The energy optimization is based on the stochastic reconfiguration (SR) method developed in order to optimize many parameters [25]. To stabilize the SR method, we also use a truncation technique for irrelevant variational parameters [26] and a stochastic annealing approach [17]. The scaling of the numerical complexity resulting from calculating the matrix product scales as χ^3 . Note that all the matrix elements in $\hat{A}_{[k]}^{j_k}$ of the MPPS could be the variational parameters to be optimized. However, for simplicity, we assume the matrices to be real, symmetric and translationally invariant here.

Figure 2a compares the optimized energies for Hamiltonian (4) using a $L = 18$ chain with periodic boundary condition with the exact ground-state energy E_0 . The ex-

act ground-state energies are obtained using sparse matrix diagonalization. The advantage of the MPPS approach over the regular MPS is especially clear in the regime of small V/t . Here, the $V = 0$ ground state used in the MPPS is a much better approximation of the ground state compared to the site-factorized wave function used in the MPS. Thus it pays off that part of the entanglement is already contained in $|\phi_0^{\text{Slater}}\rangle$ making the MPPS more efficient. The MPPS yields lower energies in the regime of large V/t as well, even though the advantage is less pronounced. The simple density-density repulsive Jastrow-type wave function is a good approximation of the ground states for small V/t , however, it fails to describe the gapped phases in the regime $V/t > 2$. In particular, it does not capture the phase transition to the charge ordered state at $V/t = 2$. Figure 2b shows the χ -dependence of the energies and compares the results to the exact ground-state energies E_0 in the thermodynamic limit. The energies for infinite systems are obtained using a infinite time-evolving block decimation (iTEBD) [27] algorithm using MPS with large bond dimensions ($\chi > 300$). In the gapless phase ($V/t = 1$), we find that the MPPS results show much faster convergence to the ground state than the MPS. The MPPS with $\chi = 5$ already has an energy which is very close to the ground state (error off 10^{-4}) while the MPS displays comparably slow convergence up to $\chi = 10$. Even at the critical point ($V/t = 2$), the MPPS gives significantly better results than the MPS.

In order to further test the quality of the wave function, we compute the density-density correlation function

$$C_{nn}(R) = \frac{1}{L} \sum_i \langle n_i n_{i+R} \rangle - \frac{1}{4}. \quad (8)$$

Figure 3 shows the obtained correlation function C_{nn} for the MPS and the MPPS using the same bond dimension with the exact results. The exact results are calculated using the iTEBD algorithms with large bond dimensions ($\chi > 300$). Note that to avoid the staggered decay of the correlation function arising from the $2k_F$ components, we only show the correlation function with odd sites. Let us first discuss the gapless regime shown in Fig. 3a. In the $V = 0$ case, the MPPS results are exact (up to the statistical errors) and we obtain the expected R^{-2} decay of the correlations. For finite V/t , the exponents change and the correlation function is analytically given by $C_{nn}(R) = \frac{A}{R^2} + (-1)^R \frac{B}{R^{2\kappa}}$ where A and B are non-universal constants and $\kappa^{-1} = \frac{2}{\pi} \arccos(-V/2t)$ [28]. The MPPS results agree with the exact algebraic decay over ~ 50 lattice sites while the regular MPS captures only about ~ 5 lattice sites (using the same bond dimension). In order to understand the fast convergence for the MPPS in Figure 2b, it is interesting to compare the behavior of the MPS and the MPPS at long distances in Figure 3a. The MPS contains no long range entanglement and thus the correlation functions saturates to a

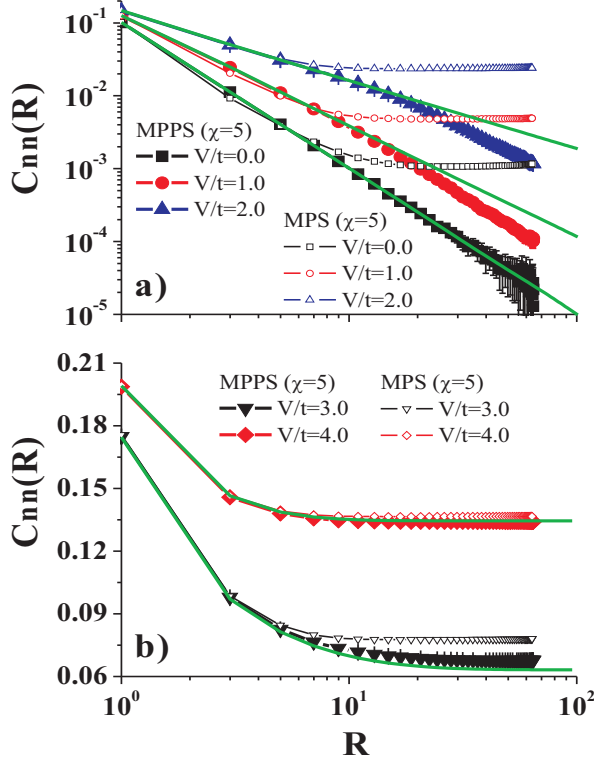


FIG. 3: (Color online) Density-density correlation function $C_{nn}(R)$ for the MPPS and the MPS with the same bond dimension as a function of distance R in a) gapless and b) CDW regions on a $L = 202$ chain. The green lines are obtained from the MPS with a large bond dimensions ($\chi > 300$) on infinite chains. For the chain with a finite length, the periodic boundary condition has been considered in the distance R .

constant as R goes to infinity. In the MPPS, we start from a free fermion wave function in which the local entanglement is modified by the matrix-product projection-operators. Thus the correlation functions fall off $\propto R^{-2}$ at long distances. This shows us intuitively why the MPPS converges faster in terms of the bond dimension χ : The matrices do not need to transform a product state into one with algebraic correlation but they only need to modify the exponent of a wave function which is already critical. In Fig. 3b, we also present the correlation function in the gapped CDW region. The CDW order parameters, enhanced as increasing V/t , can be estimated from the converged values of the correlation functions at large distance. In addition to the resemblance on the correlation functions between the MPPS and exact results, the MPPS also obtains a better estimation for the order parameter than the MPS with the same bond dimension.

The natural extension of the MPPS to two dimensions is to use tensor-product projected states (TPPS). The trial wave function is then formally written identical to Eq. (2) with the amplitudes W_{j_1, j_2, \dots, j_N} of the projections

given by a tensorial trace [29, 30]:

$$W_{j_1, j_2, \dots, j_N} = \text{tTr} \left(\hat{T}_{[1]}^{j_1} \hat{T}_{[2]}^{j_2} \dots \hat{T}_{[N]}^{j_N} \right). \quad (9)$$

Here $\hat{T}_{[k]}^{j_k}$ are rank z -tensors with z being the coordination number of the lattice and N lattice size. The tensorial trace tTr is a generalization of the matrix-trace and implies a contraction over all virtual bond indices. The main difficulty is that the tensorial trace cannot be exactly evaluated anymore. This is because the numerical effort to contract the tensors grows exponentially with the linear dimension of the systems. To overcome this problem, we can utilize several approximate ways to calculate the contraction [31, 32]. One way to approximate the trace is to use the tensor entanglement renormalization group method [32]. The numerical complexity depends then on the lattice, e.g., applied to a honeycomb lattice, and that of the approximate evaluation of the tensorial trace scales as χ^6 . The generalization of the method to two dimensions is now being studied [33].

In conclusion, we have introduced a projected wave function approach which is based on matrix-product projection-operators. The approach is as a generalization of the MPS in which the initial state is not necessarily assumed to be close to a site-factorized state. We have demonstrated that the quality of the wave functions, MPPS, is superior to the MPS with the same bond dimension by comparing energies and correlation functions for a one-dimension model of spinless fermions. The approach can be generalized to higher dimensions by using tensor-product based projection-operators. Here we expect our approach to be particularly useful because the computational complexity grows very quickly with the dimension of the tensors and thus it is very beneficial to express part of the entanglement by using a suitable initial wave function.

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